



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:40 PM GMT

PDB ID : 4M8D
Title : Crystal structure of an isatin hydrolase bound to product analogue thioisatinate
Authors : Bjerregaard-Andersen, K.; Sommer, T.; Jensen, J.K.; Jochimsen, B.; Etzerodt, M.; Morth, J.P.
Deposited on : 2013-08-13
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

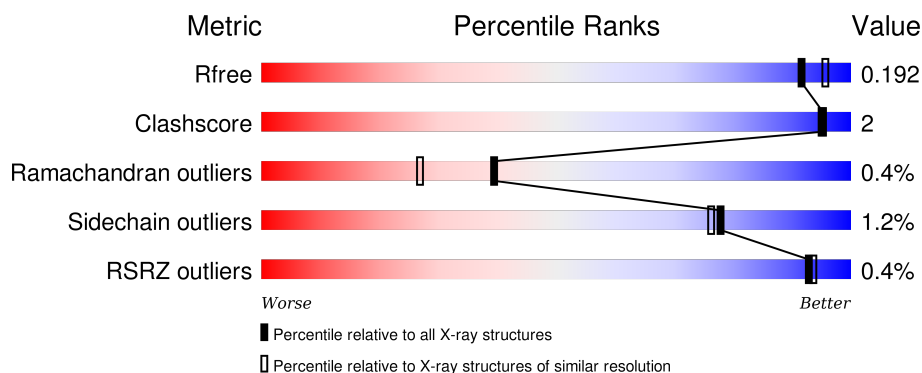
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	<div> <div></div> <div>97%</div> <div>.</div> </div>
1	B	263	<div> <div></div> <div>97%</div> <div>.</div> </div>
1	C	263	<div> <div>%</div> <div>94%</div> <div>5%</div> </div>
1	D	263	<div> <div></div> <div>96%</div> <div>.</div> </div>
1	E	263	<div> <div></div> <div>94%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	263	 97%
1	G	263	 95%
1	H	263	 94% 5%
1	I	263	 92% 7%
1	J	263	 92% 8%
1	K	263	 95%
1	L	263	 94% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	23J	A	302	-	-	-	X
3	23J	B	302[A]	-	-	-	X
3	23J	B	302[B]	-	-	-	X
3	23J	C	302	-	-	-	X
3	23J	D	302	-	-	-	X
3	23J	E	302	-	-	-	X
3	23J	F	302[A]	-	-	-	X
3	23J	F	302[B]	-	-	-	X
3	23J	G	302[A]	-	-	-	X
3	23J	G	302[B]	-	-	-	X
3	23J	H	302	-	-	-	X
3	23J	I	302	-	-	-	X
3	23J	J	302	-	-	-	X
3	23J	K	302	-	-	-	X
3	23J	L	302	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27233 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	1	0
			1978	1257	333	380	8			
1	B	262	Total	C	N	O	S	0	1	0
			1973	1254	332	380	7			
1	C	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	D	263	Total	C	N	O	S	0	0	0
			1978	1257	333	380	8			
1	E	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	F	263	Total	C	N	O	S	0	0	0
			1977	1257	333	379	8			
1	G	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	H	263	Total	C	N	O	S	0	0	0
			1978	1257	333	380	8			
1	I	262	Total	C	N	O	S	0	1	0
			1980	1259	335	378	8			
1	J	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	K	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	L	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

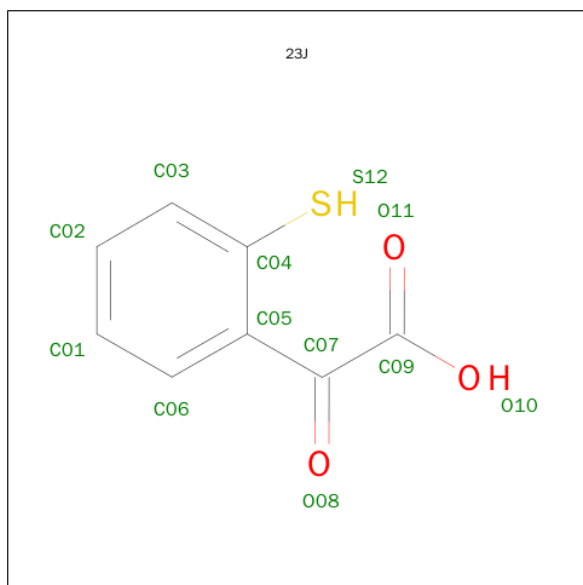
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	J	1	Total	Mn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mn	0	0
			1	1		
2	K	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	I	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	L	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is OXO(2-SULFANYLPHENYL)ACETIC ACID (three-letter code: 23J) (formula: C₈H₆O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			12	8	3	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	1
			24	16	6	2		
3	C	1	Total	C	O	S	0	0
			12	8	3	1		
3	D	1	Total	C	O	S	0	0
			12	8	3	1		
3	E	1	Total	C	O	S	0	0
			12	8	3	1		
3	F	1	Total	C	O	S	0	1
			24	16	6	2		
3	G	1	Total	C	O	S	0	1
			24	16	6	2		
3	H	1	Total	C	O	S	0	0
			12	8	3	1		
3	I	1	Total	C	O	S	0	0
			12	8	3	1		
3	J	1	Total	C	O	S	0	0
			12	8	3	1		
3	K	1	Total	C	O	S	0	0
			12	8	3	1		
3	L	1	Total	C	O	S	0	0
			12	8	3	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	2	Total	Ca	0	0
			2	2		
4	D	1	Total	Ca	0	0
			1	1		
4	B	3	Total	Ca	0	0
			3	3		
4	I	1	Total	Ca	0	0
			1	1		
4	C	2	Total	Ca	0	0
			2	2		
4	A	3	Total	Ca	0	0
			3	3		
4	L	3	Total	Ca	0	0
			3	3		
4	F	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

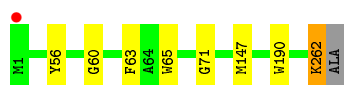
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	318	Total	O	0	0
			318	318		
5	B	323	Total	O	0	0
			323	323		
5	C	237	Total	O	0	0
			237	237		
5	D	293	Total	O	0	0
			293	293		
5	E	266	Total	O	0	0
			266	266		
5	F	320	Total	O	0	0
			320	320		
5	G	240	Total	O	0	0
			240	240		
5	H	237	Total	O	0	0
			237	237		
5	I	282	Total	O	0	0
			282	282		
5	J	259	Total	O	0	0
			259	259		
5	K	279	Total	O	0	0
			279	279		
5	L	275	Total	O	0	0
			275	275		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

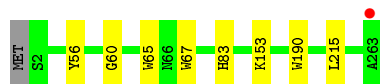
- Molecule 1: Putative uncharacterized protein

Chain A:  97%



- Molecule 1: Putative uncharacterized protein

Chain B:  97%



- Molecule 1: Putative uncharacterized protein

Chain C:  94% 5%



- Molecule 1: Putative uncharacterized protein

Chain D:  96%



- Molecule 1: Putative uncharacterized protein

Chain E:  94% 5%



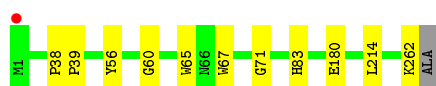
- Molecule 1: Putative uncharacterized protein

Chain F:  97%



- Molecule 1: Putative uncharacterized protein

Chain G:  95%




- Molecule 1: Putative uncharacterized protein

Chain H:  94% 5%



- Molecule 1: Putative uncharacterized protein

Chain I:  92% 7%



- Molecule 1: Putative uncharacterized protein

Chain J:  92% 8%



- Molecule 1: Putative uncharacterized protein

Chain K:  95%



- Molecule 1: Putative uncharacterized protein

Chain L:  94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.98Å 51.82Å 357.09Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	29.98 – 1.90 49.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.98-1.90) 97.6 (49.51-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.152 , 0.192 0.154 , 0.192	Depositor DCC
R_{free} test set	12062 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.1	EDS
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 282748 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27233	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.76 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.4828e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MN, 23J

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/2032	0.54	0/2772
1	B	0.40	0/2030	0.54	0/2769
1	C	0.33	0/2026	0.50	0/2764
1	D	0.39	0/2032	0.55	0/2771
1	E	0.39	0/2026	0.54	0/2764
1	F	0.39	0/2031	0.54	0/2771
1	G	0.36	0/2026	0.51	0/2764
1	H	0.35	0/2032	0.50	0/2771
1	I	0.37	0/2037	0.54	0/2778
1	J	0.38	0/2026	0.53	0/2764
1	K	0.37	0/2026	0.52	0/2764
1	L	0.38	0/2026	0.51	0/2764
All	All	0.38	0/24350	0.53	0/33216

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1978	0	1922	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1973	0	1915	4	0
1	C	1972	0	1918	7	0
1	D	1978	0	1923	5	0
1	E	1972	0	1918	10	0
1	F	1977	0	1923	4	0
1	G	1972	0	1918	5	0
1	H	1978	0	1923	9	0
1	I	1980	0	1931	11	0
1	J	1972	0	1918	14	0
1	K	1972	0	1918	6	0
1	L	1972	0	1918	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	12	0	5	0	0
3	B	24	0	10	3	0
3	C	12	0	5	2	0
3	D	12	0	5	1	0
3	E	12	0	5	1	0
3	F	24	0	10	4	0
3	G	24	0	10	1	0
3	H	12	0	5	1	0
3	I	12	0	5	1	0
3	J	12	0	5	1	0
3	K	12	0	5	2	0
3	L	12	0	5	1	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	3	0	0	0	0
5	A	318	0	0	1	0
5	B	323	0	0	0	0
5	C	237	0	0	1	0
5	D	293	0	0	0	0
5	E	266	0	0	0	0
5	F	320	0	0	0	0
5	G	240	0	0	0	0
5	H	237	0	0	0	0
5	I	282	0	0	1	0
5	J	259	0	0	0	0
5	K	279	0	0	1	0
5	L	275	0	0	0	0
All	All	27233	0	23120	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:HIS:NE2	3:B:302[B]:23J:O10	2.14	0.79
1:A:262:LYS:O	5:A:711:HOH:O	2.12	0.67
1:F:83:HIS:NE2	3:F:302[A]:23J:O11	2.31	0.63
1:E:63:PHE:CE1	3:F:302[B]:23J:H1	2.35	0.62
1:C:83:HIS:NE2	3:C:302:23J:O11	2.33	0.61
1:K:83:HIS:NE2	3:K:302:23J:O10	2.34	0.60
1:G:67:TRP:HA	1:H:71:GLY:HA2	1.84	0.59
1:I:146:VAL:HG13	1:I:229:LEU:HD13	1.85	0.58
1:B:153:LYS:HD2	1:D:16:SER:HB2	1.86	0.58
1:L:83:HIS:NE2	3:L:302:23J:O11	2.36	0.58
1:K:138:GLU:OE1	1:K:185:LYS:NZ	2.32	0.56
3:C:302:23J:O10	5:C:469:HOH:O	2.18	0.56
1:H:180:GLU:HG2	1:H:214:LEU:HD13	1.88	0.56
1:I:67:TRP:HA	1:J:71:GLY:HA2	1.88	0.55
1:J:176:PRO:HD3	1:J:205:MET:HE2	1.90	0.54
1:E:1:MET:N	1:E:2:SER:HA	2.22	0.54
1:K:261:PRO:O	1:K:262:LYS:HB2	2.07	0.54
1:I:261:PRO:O	1:I:262:LYS:HB2	2.07	0.53
1:E:83:HIS:NE2	3:E:302:23J:O10	2.42	0.53
1:J:180:GLU:HG2	1:J:214:LEU:HD13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:GLY:HA2	1:J:67:TRP:HA	1.92	0.52
1:D:83:HIS:NE2	3:D:302:23J:O10	2.43	0.52
1:J:202:ALA:HA	1:J:205:MET:SD	2.51	0.51
1:L:180:GLU:HG3	1:L:214:LEU:HD13	1.93	0.51
1:J:176:PRO:HD3	1:J:205:MET:CE	2.41	0.50
3:K:302:23J:O11	5:K:679:HOH:O	2.19	0.50
1:H:198:ASP:HB3	1:H:202:ALA:HB2	1.92	0.50
1:L:202:ALA:HA	1:L:205:MET:HG3	1.94	0.49
1:E:63:PHE:CD1	3:F:302[B]:23J:H1	2.46	0.49
1:C:70:LEU:HD21	1:C:253:PRO:HG3	1.93	0.49
1:A:63:PHE:CD1	3:B:302[A]:23J:H1	2.47	0.48
1:C:67:TRP:HA	1:D:71:GLY:HA2	1.95	0.48
1:I:13:LYS:HE2	1:J:1:MET:HG3	1.96	0.48
1:G:83:HIS:NE2	3:G:302[B]:23J:O11	2.46	0.47
1:H:83:HIS:NE2	3:H:302:23J:O10	2.47	0.47
1:I:1:MET:HA	1:I:2:SER:HA	1.58	0.47
1:H:202:ALA:HB1	1:H:209:PHE:HA	1.97	0.46
1:L:261:PRO:O	1:L:262:LYS:HB3	2.15	0.46
1:L:172:PRO:HD2	1:L:194:CYS:SG	2.55	0.46
1:E:67:TRP:HA	1:F:71:GLY:HA2	1.97	0.46
1:B:190:TRP:HB3	1:B:215:LEU:HD11	1.98	0.46
1:H:172:PRO:HD2	1:H:194:CYS:SG	2.56	0.46
1:I:83:HIS:NE2	3:I:302:23J:O11	2.49	0.45
1:C:172:PRO:HD2	1:C:194:CYS:SG	2.56	0.45
1:J:83:HIS:NE2	3:J:302:23J:O10	2.50	0.45
1:I:25:THR:HG23	1:I:76:THR:HB	1.97	0.44
1:E:190:TRP:HB3	1:E:215:LEU:HD11	1.99	0.44
1:K:71:GLY:HA2	1:L:67:TRP:HA	1.98	0.44
1:E:147:MET:HB2	1:E:190:TRP:CH2	2.52	0.44
1:C:262:LYS:HD3	1:C:262:LYS:HA	1.63	0.44
1:G:71:GLY:HA2	1:H:67:TRP:HA	2.00	0.44
1:A:63:PHE:CE1	3:B:302[A]:23J:H1	2.53	0.44
1:C:190:TRP:HB3	1:C:215:LEU:HD11	1.99	0.44
1:J:175:THR:OG1	1:J:177:ASP:OD1	2.26	0.44
5:I:533:HOH:O	1:J:1:MET:SD	2.62	0.44
1:E:3:ALA:HB2	1:F:18:GLU:HG2	1.99	0.44
1:J:261:PRO:O	1:J:262:LYS:HB2	2.17	0.44
1:D:260:VAL:HG23	1:D:262:LYS:HD3	2.01	0.43
1:G:180:GLU:HG2	1:G:214:LEU:HD13	1.99	0.43
1:J:15:LEU:HA	1:J:15:LEU:HD12	1.81	0.43
1:I:38:PRO:HA	1:I:39:PRO:HD3	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:147:MET:HB2	1:J:190:TRP:CH2	2.55	0.42
1:L:190:TRP:HB3	1:L:215:LEU:HD11	2.01	0.41
1:A:71:GLY:HA2	1:B:67:TRP:HA	2.03	0.41
1:G:38:PRO:HA	1:G:39:PRO:HD3	1.97	0.41
1:A:147:MET:HB2	1:A:190:TRP:CH2	2.55	0.41
1:D:84:TRP:CD2	1:D:212:HIS:HB3	2.56	0.41
1:K:70:LEU:HD21	1:K:253:PRO:HG2	2.03	0.41
1:C:90:TYR:CZ	1:C:219:ASN:HB2	2.56	0.41
1:H:20:GLU:OE1	1:H:262:LYS:HE3	2.21	0.41
1:I:10:LEU:HD22	1:J:10:LEU:HD22	2.02	0.41
1:F:149:THR:HG21	1:F:172:PRO:HG2	2.03	0.40
1:K:13:LYS:NZ	1:L:1:MET:O	2.47	0.40
1:E:63:PHE:CZ	3:F:302[B]:23J:H1	2.55	0.40
1:I:262:LYS:HE3	1:I:262:LYS:HB3	1.87	0.40
1:E:180:GLU:HG2	1:E:214:LEU:HD13	2.02	0.40
1:H:65:TRP:N	1:H:65:TRP:CD1	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	39	27
1	B	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	39	27
1	C	260/263 (99%)	252 (97%)	7 (3%)	1 (0%)	39	27
1	D	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	39	27
1	E	260/263 (99%)	256 (98%)	3 (1%)	1 (0%)	39	27
1	F	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	39	27
1	G	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	39	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	39	27
1	I	261/263 (99%)	255 (98%)	5 (2%)	1 (0%)	39	27
1	J	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	39	27
1	K	260/263 (99%)	254 (98%)	5 (2%)	1 (0%)	39	27
1	L	260/263 (99%)	254 (98%)	5 (2%)	1 (0%)	39	27
All	All	3125/3156 (99%)	3060 (98%)	53 (2%)	12 (0%)	39	27

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	60	GLY
1	J	60	GLY
1	A	60	GLY
1	B	60	GLY
1	D	60	GLY
1	E	60	GLY
1	K	60	GLY
1	C	60	GLY
1	G	60	GLY
1	H	60	GLY
1	L	60	GLY
1	F	60	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/207 (100%)	205 (99%)	3 (1%)	74	71
1	B	207/207 (100%)	205 (99%)	2 (1%)	82	81
1	C	207/207 (100%)	204 (99%)	3 (1%)	74	71
1	D	207/207 (100%)	205 (99%)	2 (1%)	82	81
1	E	207/207 (100%)	203 (98%)	4 (2%)	65	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	207/207 (100%)	205 (99%)	2 (1%)	82	81
1	G	207/207 (100%)	204 (99%)	3 (1%)	74	71
1	H	207/207 (100%)	205 (99%)	2 (1%)	82	81
1	I	208/207 (100%)	203 (98%)	5 (2%)	57	49
1	J	207/207 (100%)	205 (99%)	2 (1%)	82	81
1	K	207/207 (100%)	206 (100%)	1 (0%)	92	92
1	L	207/207 (100%)	205 (99%)	2 (1%)	82	81
All	All	2486/2484 (100%)	2455 (99%)	31 (1%)	78	76

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	TYR
1	A	65	TRP
1	A	262	LYS
1	B	56	TYR
1	B	65	TRP
1	C	56	TYR
1	C	65	TRP
1	C	262	LYS
1	D	56	TYR
1	D	65	TRP
1	E	1	MET
1	E	56	TYR
1	E	65	TRP
1	E	262	LYS
1	F	56	TYR
1	F	65	TRP
1	G	56	TYR
1	G	65	TRP
1	G	262	LYS
1	H	56	TYR
1	H	65	TRP
1	I	56	TYR
1	I	65	TRP
1	I	146	VAL
1	I	248[A]	ARG
1	I	248[B]	ARG
1	J	40	ASP
1	J	65	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	65	TRP
1	L	56	TYR
1	L	65	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 43 ligands modelled in this entry, 28 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	23J	A	302	2	9,12,12	0.43	0	9,16,16	0.90	1 (11%)
3	23J	B	302[A]	-	9,12,12	0.45	0	9,16,16	0.74	0
3	23J	B	302[B]	2	9,12,12	0.47	0	9,16,16	0.97	1 (11%)
3	23J	C	302	2	9,12,12	0.34	0	9,16,16	0.86	0
3	23J	D	302	2	9,12,12	0.47	0	9,16,16	0.86	0
3	23J	E	302	2	9,12,12	0.34	0	9,16,16	1.07	1 (11%)
3	23J	F	302[A]	2	9,12,12	0.48	0	9,16,16	1.02	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	23J	F	302[B]	-	9,12,12	0.68	0	9,16,16	0.93	1 (11%)
3	23J	G	302[A]	-	9,12,12	0.33	0	9,16,16	0.63	0
3	23J	G	302[B]	2	9,12,12	0.47	0	9,16,16	0.74	0
3	23J	H	302	2	9,12,12	0.44	0	9,16,16	1.00	1 (11%)
3	23J	I	302	2	9,12,12	0.62	0	9,16,16	0.78	0
3	23J	J	302	2	9,12,12	0.44	0	9,16,16	1.14	1 (11%)
3	23J	K	302	2	9,12,12	0.39	0	9,16,16	0.92	1 (11%)
3	23J	L	302	2	9,12,12	0.37	0	9,16,16	0.96	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	23J	A	302	2	-	0/4/8/8	0/1/1/1
3	23J	B	302[A]	-	-	0/4/8/8	0/1/1/1
3	23J	B	302[B]	2	-	0/4/8/8	0/1/1/1
3	23J	C	302	2	-	0/4/8/8	0/1/1/1
3	23J	D	302	2	-	0/4/8/8	0/1/1/1
3	23J	E	302	2	-	0/4/8/8	0/1/1/1
3	23J	F	302[A]	2	-	0/4/8/8	0/1/1/1
3	23J	F	302[B]	-	-	0/4/8/8	0/1/1/1
3	23J	G	302[A]	-	-	0/4/8/8	0/1/1/1
3	23J	G	302[B]	2	-	0/4/8/8	0/1/1/1
3	23J	H	302	2	-	0/4/8/8	0/1/1/1
3	23J	I	302	2	-	0/4/8/8	0/1/1/1
3	23J	J	302	2	-	0/4/8/8	0/1/1/1
3	23J	K	302	2	-	0/4/8/8	0/1/1/1
3	23J	L	302	2	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	302	23J	O08-C07-C05	2.04	123.62	119.81
3	A	302	23J	O08-C07-C05	2.06	123.65	119.81
3	F	302[A]	23J	O08-C07-C05	2.11	123.75	119.81
3	L	302	23J	O08-C07-C05	2.12	123.77	119.81
3	F	302[B]	23J	C05-C07-C09	2.13	122.89	119.24
3	B	302[B]	23J	O08-C07-C05	2.15	123.82	119.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	23J	O08-C07-C05	2.40	124.29	119.81
3	H	302	23J	O08-C07-C05	2.54	124.54	119.81
3	J	302	23J	O08-C07-C05	2.61	124.68	119.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302[A]	23J	2	0
3	B	302[B]	23J	1	0
3	C	302	23J	2	0
3	D	302	23J	1	0
3	E	302	23J	1	0
3	F	302[A]	23J	1	0
3	F	302[B]	23J	3	0
3	G	302[B]	23J	1	0
3	H	302	23J	1	0
3	I	302	23J	1	0
3	J	302	23J	1	0
3	K	302	23J	2	0
3	L	302	23J	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	262/263 (99%)	-0.65	1 (0%) 93 93	10, 18, 33, 65	0
1	B	262/263 (99%)	-0.63	1 (0%) 93 93	9, 20, 34, 57	0
1	C	262/263 (99%)	-0.43	2 (0%) 87 88	16, 29, 45, 92	0
1	D	263/263 (100%)	-0.54	1 (0%) 93 93	13, 21, 40, 99	0
1	E	262/263 (99%)	-0.62	1 (0%) 93 93	11, 21, 37, 119	0
1	F	263/263 (100%)	-0.62	1 (0%) 93 93	11, 19, 36, 71	0
1	G	262/263 (99%)	-0.53	1 (0%) 93 93	15, 25, 41, 86	0
1	H	263/263 (100%)	-0.38	2 (0%) 87 88	15, 28, 44, 94	0
1	I	262/263 (99%)	-0.60	1 (0%) 93 93	13, 22, 36, 88	0
1	J	262/263 (99%)	-0.62	0 100 100	13, 22, 36, 54	0
1	K	262/263 (99%)	-0.59	1 (0%) 93 93	14, 23, 38, 104	0
1	L	262/263 (99%)	-0.65	1 (0%) 93 93	13, 21, 35, 67	0
All	All	3147/3156 (99%)	-0.57	13 (0%) 93 93	9, 22, 40, 119	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	1	MET	9.2
1	G	1	MET	9.0
1	E	1	MET	8.2
1	F	1	MET	7.0
1	I	1	MET	6.8
1	D	1	MET	6.4
1	H	1	MET	5.1
1	H	263	ALA	4.8
1	C	1	MET	4.6
1	A	1	MET	4.1
1	L	1	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	263	ALA	2.3
1	C	41	PHE	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	23J	F	302[A]	12/12	0.81	0.19	13.20	21,29,31,42	12
3	23J	I	302	12/12	0.86	0.21	10.80	35,37,42,117	12
3	23J	B	302[B]	12/12	0.88	0.22	10.20	24,32,33,112	12
3	23J	D	302	12/12	0.90	0.17	10.17	28,31,42,101	12
3	23J	F	302[B]	12/12	0.81	0.19	10.08	16,29,31,39	12
3	23J	G	302[B]	12/12	0.84	0.25	9.69	37,45,45,156	12
3	23J	H	302	12/12	0.84	0.21	8.97	36,39,43,158	12
3	23J	E	302	12/12	0.89	0.16	7.53	32,36,40,103	12
3	23J	G	302[A]	12/12	0.84	0.25	6.85	43,45,47,156	12
3	23J	K	302	12/12	0.90	0.15	5.97	26,29,36,67	12
3	23J	C	302	12/12	0.85	0.17	5.94	39,40,52,83	12
3	23J	B	302[A]	12/12	0.88	0.22	5.73	31,33,35,112	12
3	23J	A	302	12/12	0.94	0.16	5.53	33,34,45,136	0
3	23J	J	302	12/12	0.90	0.14	4.78	32,35,40,140	12
3	23J	L	302	12/12	0.91	0.12	4.45	31,35,41,152	0
2	MN	K	301	1/1	0.98	0.07	-0.10	20,20,20,20	0
4	CA	I	303	1/1	0.98	0.07	-0.75	21,21,21,21	0
4	CA	L	305	1/1	0.95	0.07	-0.76	47,47,47,47	0
4	CA	F	303	1/1	0.99	0.06	-1.08	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	J	304	1/1	0.96	0.05	-1.65	50,50,50,50	0
4	CA	B	305	1/1	0.95	0.05	-2.25	43,43,43,43	0
4	CA	C	303	1/1	0.97	0.05	-2.59	31,31,31,31	0
4	CA	B	304	1/1	0.99	0.05	-3.06	23,23,23,23	0
2	MN	G	301	1/1	0.99	0.04	-3.90	22,22,22,22	0
4	CA	L	303	1/1	0.99	0.03	-5.30	23,23,23,23	0
4	CA	J	303	1/1	0.99	0.04	-5.35	26,26,26,26	0
4	CA	C	304	1/1	0.63	0.17	-	81,81,81,81	0
2	MN	L	301	1/1	0.99	0.05	-	17,17,17,17	0
2	MN	E	301	1/1	0.99	0.05	-	15,15,15,15	0
2	MN	A	301	1/1	0.99	0.07	-	14,14,14,14	0
4	CA	A	305	1/1	0.94	0.10	-	52,52,52,52	0
4	CA	L	304	1/1	0.98	0.05	-	35,35,35,35	0
4	CA	D	303	1/1	0.97	0.07	-	46,46,46,46	0
2	MN	J	301	1/1	0.99	0.04	-	18,18,18,18	0
2	MN	F	301	1/1	0.99	0.06	-	16,16,16,16	0
4	CA	A	303	1/1	0.95	0.08	-	36,36,36,36	0
2	MN	C	301	1/1	0.96	0.06	-	22,22,22,22	0
2	MN	B	301	1/1	0.99	0.05	-	17,17,17,17	0
2	MN	I	301	1/1	0.99	0.04	-	16,16,16,16	0
2	MN	H	301	1/1	0.96	0.05	-	24,24,24,24	0
2	MN	D	301	1/1	0.99	0.06	-	18,18,18,18	0
4	CA	B	303	1/1	0.94	0.06	-	34,34,34,34	0
4	CA	A	304	1/1	0.99	0.04	-	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.